

RESEARCHERS

26

STAFF SCIENTISTS

50

STUDENTS

INVITED TALKS

122

FY 2014 - 2016

FELLOWS

14



Creating Materials & Energy Solutions
U.S. DEPARTMENT OF ENERGY

CHEMICAL AND BIOLOGICAL SCIENCES

BY THE NUMBERS

PAPERS

94

PUBLISHED

540

CITATIONS

FY 2014 - 2016
citations as of Mar. 2017

PATENTS

4

FILED

3

ISSUED

FY 2014- 2016

COLLABORATING INSTITUTIONS

70

FY 2014 - 2016

TOP TEN PAPERS

- 1 Shape Evolution and Single Particle Luminescence of Organometal Halide Perovskite Nanocrystals, *ACS Nano*, 2015, 9, pp 2948-2959
- 2 Natural Abundance O-17 DNP Two-Dimensional and Surface-Enhanced NMR Spectroscopy, *Journal of the American Chemical Society*, 2015, 137, pp 8336-8339
- 3 Six Questions on Topology in Theoretical Chemistry, *Computational and Theoretical Chemistry*, 2015, 1053, pp 2-16
- 4 Dynamic Nuclear Polarization Solid-State NMR in Heterogeneous Catalysis Research, *ACS Catalysis*, 2015, 5, pp 7055-7062
- 5 Zirconium-Catalyzed Desymmetrization of Aminodialkenes and Aminodialkynes through Enantioselective Hydroamination, *Journal of the American Chemical Society*, 2015, 137, pp 425-435
- 6 Analytic Gradient for Density Functional Theory Based on the Fragment Molecular Orbital Method, *Journal of Chemical Theory and Computation*, 2014, 10, pp 5297-5307
- 7 Benzene Selectivity in Competitive Arene Hydrogenation: Effects of Single-Site Catalyst - Acidic Oxide Surface Binding Geometry, *Journal of the American Chemical Society*, 2015, 137, pp 6770-6780
- 8 Studies of Minute Quantities of Natural Abundance Molecules Using 2D Heteronuclear Correlation Spectroscopy Under 100 kHz MAS, *Solid State Nuclear Magnetic Resonance*, 2015, pp 56-61
- 9 Cu₂S₃ complex on Cu(111) as a Candidate for Mass Transport Enhancement, *Physical Review B*, 2015, 91, 045426
- 10 Real-Time Ab Initio KMC Simulation of the Self-Assembly and Sintering of Bimetallic Epitaxial Nanoclusters: Au + Ag on Ag(100), *Nano Letters*, 2014, 14, pp 4646-4652

FY 2014 - 2016, citations as of Mar. 2017